STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 175938

TO: Mary K Zeman **Location: REM/2D61/2C70** **Art Unit: 1631** **Thursday, January 19, 2006** **Case Serial Number: 10/655870**	**From: Mary Jane Ruhl** **Location: Biotech-Chem Library** **Remsen 1-A-62** **Phone: 571-272-2524** **maryjane.ruhl@uspto.gov**

Search Notes

Examiner Zeman,

Here are the results for your recent search request.

Filed 9/5/03
No Prov/Priority

Please feel free to contact me if you have any questions about these results.

Thank you for using STIC services. We appreciate the opportunity to serve you.

1/27/04 OK
new drawings
4/7/04
IDS

Sincerely,

Mary Jane Ruhl
Technical Information Specialist
STIC
Remsen 1-A-62
Ext. 22524

Purvis, G

Claims 1-10, 31
System, no hardware 101
Not concrete, tangible, useful

11-20
Method. Not CTU, 101

21-30
Software embodied.

31 - means + function
System 112
No hardware
Structure in Spec?

```
=> d his ful

     (FILE 'HOME' ENTERED AT 17:54:45 ON 19 JAN 2006)

     FILE 'HCAPLUS' ENTERED AT 17:54:53 ON 19 JAN 2006
                E PURVIS GEORGE
                E PURVIS GEORGE/AU
L1           73 SEA ABB=ON  ("PURVIS G G"/AU OR "PURVIS G H"/AU OR "PURVIS
                GEORGE"/AU OR "PURVIS GEORGE A"/AU OR "PURVIS GEORGE D"/AU OR
                "PURVIS GEORGE D III"/AU)
L2            2 SEA ABB=ON  L1 AND ?PROTEIN?(W)?LIGAND?
L3              ANALYZE L2 1-1 CT :      14 TERMS

     FILE 'HCAPLUS' ENTERED AT 18:01:51 ON 19 JAN 2006
L4         1965 SEA ABB=ON  ?POTENTIAL?(3W)?MEAN?(W)?FORCE? OR PMF
L5           26 SEA ABB=ON  L4 AND ?PROTEIN?(W)?LIGAND?
L6            4 SEA ABB=ON  L5 AND (?REPULS? OR ?PAIR? OR ?INTERATOM?)(W)?POTEN
                T?
L7            2 SEA ABB=ON  L6 AND (PRD<20030905 OR PD<20030905)

     FILE 'MEDLINE, BIOSIS, EMBASE, JAPIO, JICST-EPLUS, COMPENDEX' ENTERED AT
     18:04:25 ON 19 JAN 2006
L8            3 SEA ABB=ON  L6
L9            1 DUP REMOV L8 (2 DUPLICATES REMOVED)

     FILE 'USPATFULL' ENTERED AT 18:05:53 ON 19 JAN 2006
L10           3 SEA ABB=ON  L6 AND (PRD<20030905 OR PD<20030905)

     FILE HOME

     FILE HCAPLUS

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     FILE COVERS 1907 - 19 Jan 2006  VOL 144 ISS 4
     FILE LAST UPDATED: 18 Jan 2006  (20060118/ED)

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

      This file contains CAS Registry Numbers for easy and accurate
      substance identification.

     FILE MEDLINE
      FILE LAST UPDATED: 19 JAN 2006 (20060119/UP).  FILE COVERS 1950 TO DATE.

      On December 11, 2005, the 2006 MeSH terms were loaded.

      The MEDLINE reload for 2006 will soon be available.  For details
      on the 2005 reload, enter HELP RLOAD at an arrow promt (=>).
      See also:

         http://www.nlm.nih.gov/mesh/
```

http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html
http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_med_data_changes.html
http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_2006_MeSH.html

OLDMEDLINE is covered back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2006 vocabulary.

This file contains CAS Registry Numbers for easy and accurate

FILE BIOSIS
FILE COVERS 1969 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 19 January 2006 (20060119/ED)

FILE EMBASE
FILE COVERS 1974 TO 12 Jan 2006 (20060112/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE JAPIO
FILE LAST UPDATED: 02 JAN 2006 <20060102/UP>
FILE COVERS APR 1973 TO SEPTEMBER 29, 2005

>>> GRAPHIC IMAGES AVAILABLE <<<

>>> NEW IPC8 DATA AND FUNCTIONALITY NOT YET AVAILABLE IN THIS FILE. USE IPC7 FORMAT FOR SEARCHING THE IPC. WATCH THIS SPACE FOR FURTHER DEVELOPMENTS AND SEE OUR NEWS SECTION FOR FURTHER INFORMATION ABOUT THE IPC REFORM <<<

FILE JICST-EPLUS
FILE COVERS 1985 TO 18 JAN 2006 (20060118/ED)

THE JICST-EPLUS FILE HAS BEEN RELOADED TO REFLECT THE 1999 CONTROLLED TERM (/CT) THESAURUS RELOAD.

FILE COMPENDEX
FILE LAST UPDATED: 16 JAN 2006 <20060116/UP>
FILE COVERS 1970 TO DATE.

<<< SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN THE BASIC INDEX >>>

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 19 Jan 2006 (20060119/PD)
FILE LAST UPDATED: 19 Jan 2006 (20060119/ED)
HIGHEST GRANTED PATENT NUMBER: US6988280
HIGHEST APPLICATION PUBLICATION NUMBER: US2006015978
CA INDEXING IS CURRENT THROUGH 19 Jan 2006 (20060119/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 19 Jan 2006 (20060119/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

```
=> d que stat l7
L4          1965 SEA FILE=HCAPLUS ABB=ON  ?POTENTIAL?(3W)?MEAN?(W)?FORCE? OR
                 PMF
L5            26 SEA FILE=HCAPLUS ABB=ON  L4 AND ?PROTEIN?(W)?LIGAND?
L6             4 SEA FILE=HCAPLUS ABB=ON  L5 AND (?REPULS? OR ?PAIR? OR
                 ?INTERATOM?)(W)?POTENT?
L7             2 SEA FILE=HCAPLUS ABB=ON  L6 AND (PRD<20030905 OR PD<20030905)

=> d ibib abs l7 1-2

L7   ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        1999:475033  HCAPLUS
DOCUMENT NUMBER:         131:254599
TITLE:                   BLEEP-potential of mean
                         force describing protein-
                         ligand interactions: I. Generating potential
AUTHOR(S):               Mitchell, John B. O.; Laskowski, Roman A.; Alex,
                         Alexander; Thornton, Janet M.
CORPORATE SOURCE:        Department of Biochemistry and Molecular Biology,
                         University College London, London, WC1H 0AJ, UK
SOURCE:                  Journal of Computational Chemistry (1999),
                         20(11), 1165-1176
                         CODEN: JCCHDD; ISSN: 0192-8651
PUBLISHER:               John Wiley & Sons, Inc.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB   We have developed BLEEP (biomol. ligand energy evaluation protocol), an
     atomic level potential of mean force (
     PMF) describing protein-ligand interactions.
     The pair potentials for BLEEP have been derived from
     high-resolution x-ray structures of protein-ligand
     complexes in the Brookhaven Protein Data Bank (PDB), with a careful
     treatment of homol.  The use of a broad variety of protein-
     ligand structures in the derivation phase gives BLEEP more general
     applicability than previous potentials, which have been based on limited
     classes of complexes, and thus represents a significant step forward.  We
     calculate the distance distributions in protein-ligand
     interactions for all 820 possible pairs that can be chosen from our set of
     40 different atom types, including polar hydrogen.  We then use a reverse
     Boltzmann methodol. to convert these into energy-like pair
     potential functions.  Two versions of BLEEP are calculated, one
     including and one excluding interactions between protein and water.  The
     pair potentials are found to have the expected forms;
     polar and hydrogen bonding interactions show min. at short range, around
     3.0 A, whereas a typical hydrophobic interaction is repulsive at this
     distance, with values above 4.0 A being preferred.
REFERENCE COUNT:         37    THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7   ANSWER 2 OF 2  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        1999:122707  HCAPLUS
DOCUMENT NUMBER:         130:320363
TITLE:                   A General and Fast Scoring Function for
                         Protein-Ligand Interactions: A
                         Simplified Potential Approach
AUTHOR(S):               Muegge, Ingo; Martin, Yvonne C.
CORPORATE SOURCE:        Pharmaceutical Products Division, Abbott Laboratories,
                         Abbott Park, IL, 60064-6100, USA
SOURCE:                  Journal of Medicinal Chemistry (1999),
                         42(5), 791-804
```

CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A fast, simplified potential-based approach is presented that ests. the **protein-ligand** binding affinity based on the given 3D structure of a **protein-ligand** complex. This general, knowledge-based approach exploits structural information of known **protein-ligand** complexes extracted from the Brookhaven Protein Data Bank and converts it into distance-dependent Helmholtz free interaction energies of **protein-ligand** atom **pairs** (**potentials** of **mean force**, **PMF**). The definition of an appropriate reference state and the introduction of a correction term accounting for the volume taken by the ligand were found to be crucial for deriving the relevant interaction potentials that treat solvation and entropic contributions implicitly. A significant correlation between exptl. binding affinities and computed score was found for sets of diverse **protein-ligand** complexes and for sets of different ligands bound to the same target. For 77 **protein-ligand** complexes taken from the Brookhaven Protein Data Bank, the calculated score showed a standard deviation from observed binding affinities of 1.8 log Ki units and an R2 value of 0.61. The best results were obtained for the subset of 16 serine protease complexes with a standard deviation of 1.0 log Ki unit and an R2 value of 0.86. A set of 33 inhibitors modeled into a crystal structure of HIV-1 protease yielded a standard deviation of 0.8 log Ki units from measured inhibition consts. and an R2 value of 0.74. In contrast to empirical scoring functions that show similar or sometimes better correlation with observed binding affinities, our method does not involve deriving specific parameters that fit the observed binding affinities of **protein-ligand** complexes of a given training set. We compared the performance of the **PMF** score, Bohm's score (LUDI), and the SMOG score for eight different test sets of **protein-ligand** complexes. It was found that for the majority of test sets the **PMF** score performs best. The strength of the new approach presented here lies in its generality as no knowledge about measured binding affinities is needed to derive atomic interaction potentials. The use of the new scoring function in docking studies is outlined.

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> d que stat l9
L4          1965 SEA FILE=HCAPLUS ABB=ON  ?POTENTIAL?(3W)?MEAN?(W)?FORCE? OR
                 PMF
L5            26 SEA FILE=HCAPLUS ABB=ON  L4 AND ?PROTEIN?(W)?LIGAND?
L6             4 SEA FILE=HCAPLUS ABB=ON  L5 AND (?REPULS? OR ?PAIR? OR
                 ?INTERATOM?)(W)?POTENT?
L8             3 SEA L6
L9             1 DUP REMOV L8 (2 DUPLICATES REMOVED)

=> d ibib abs l9 1-1

L9   ANSWER 1 OF 1     MEDLINE on STN                    DUPLICATE 1
ACCESSION NUMBER:   1999173934     MEDLINE
DOCUMENT NUMBER:    PubMed ID: 10072678
TITLE:              A general and fast scoring function for protein-
                    ligand interactions: a simplified potential
                    approach.
AUTHOR:             Muegge I; Martin Y C
CORPORATE SOURCE:   Pharmaceutical Products Division, Abbott Laboratories,
                    Abbott Park, Illinois 60064-6100, USA..
                    ingo.muegge.b@bayer.com
SOURCE:             Journal of medicinal chemistry, (1999 Mar 11) 42 (5)
                    791-804.
                    Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY:       United States
DOCUMENT TYPE:      Journal; Article; (JOURNAL ARTICLE)
LANGUAGE:           English
FILE SEGMENT:       Priority Journals; AIDS
ENTRY MONTH:        199904
ENTRY DATE:         Entered STN: 19990426
                    Last Updated on STN: 19990426
                    Entered Medline: 19990413
```

AB A fast, simplified potential-based approach is presented that estimates the **protein-ligand** binding affinity based on the given 3D structure of a **protein-ligand** complex. This general, knowledge-based approach exploits structural information of known **protein-ligand** complexes extracted from the Brookhaven Protein Data Bank and converts it into distance-dependent Helmholtz free interaction energies of **protein-ligand** atom **pairs** (**potentials** of **mean force**, **PMF**). The definition of an appropriate reference state and the introduction of a correction term accounting for the volume taken by the ligand were found to be crucial for deriving the relevant interaction potentials that treat solvation and entropic contributions implicitly. A significant correlation between experimental binding affinities and computed score was found for sets of diverse **protein-ligand** complexes and for sets of different ligands bound to the same target. For 77 **protein-ligand** complexes taken from the Brookhaven Protein Data Bank, the calculated score showed a standard deviation from observed binding affinities of 1.8 log Ki units and an R2 value of 0.61. The best results were obtained for the subset of 16 serine protease complexes with a standard deviation of 1.0 log Ki unit and an R2 value of 0.86. A set of 33 inhibitors modeled into a crystal structure of HIV-1 protease yielded a standard deviation of 0.8 log Ki units from measured inhibition constants and an R2 value of 0.74. In contrast to empirical scoring functions that show similar or sometimes better correlation with observed binding affinities, our method does not involve deriving specific parameters that fit the observed binding affinities of **protein-ligand** complexes of a given training set. We compared the performance of the **PMF** score,

Bohm's score (LUDI), and the SMOG score for eight different test sets of **protein-ligand** complexes. It was found that for the majority of test sets the **PMF** score performs best. The strength of the new approach presented here lies in its generality as no knowledge about measured binding affinities is needed to derive atomic interaction potentials. The use of the new scoring function in docking studies is outlined.

```
=> d que stat l10
L4         1965 SEA FILE=HCAPLUS ABB=ON  ?POTENTIAL?(3W)?MEAN?(W)?FORCE? OR
                PMF
L5           26 SEA FILE=HCAPLUS ABB=ON  L4 AND ?PROTEIN?(W)?LIGAND?
L6            4 SEA FILE=HCAPLUS ABB=ON  L5 AND (?REPULS? OR ?PAIR? OR
                ?INTERATOM?)(W)?POTENT?
L10           3 SEA FILE=USPATFULL ABB=ON  L6 AND (PRD<20030905 OR PD<20030905)

=> d ibib abs l10 1-3

L10  ANSWER 1 OF 3  USPATFULL on STN
ACCESSION NUMBER:       2003:189033  USPATFULL
TITLE:                  Protein design automation for protein libraries
INVENTOR(S):            Bentzien, Joerg, White Plains, NY, UNITED STATES
                        Dahiyat, Bassil I., Altadena, CA, UNITED STATES
                        Desjarlais, John R., Pasadena, CA, UNITED STATES
                        Hayes, Robert J., Pasadena, CA, UNITED STATES
                        Vielmetter, Jost, Altadena, CA, UNITED STATES

                             NUMBER        KIND    DATE
                        ---------------- ------ --------
PATENT INFORMATION:     US 2003130827      A1   20030710            <--
APPLICATION INFO.:      US 2002-218102     A1   20020812  (10)
RELATED APPLN. INFO.:   Continuation of Ser. No. US 2001-927790, filed on 10
                        Aug 2001, PENDING

                               NUMBER         DATE
                        ------------------ --------
PRIORITY INFORMATION:   US 2001-311545P    20010810 (60)            <--
                        US 2001-324899P    20010925 (60)            <--
                        US 2002-351937P    20020125 (60)            <--
                        US 2002-352103P    20020125 (60)            <--
DOCUMENT TYPE:          Utility
FILE SEGMENT:           APPLICATION
LEGAL REPRESENTATIVE:   ROBIN M. SILVA, DORSEY & WHITNEY LLP, SUITE 3400, FOUR
                        EMBARCADERO CENTER, SAN FRANCISCO, CA, 94111
NUMBER OF CLAIMS:       116
EXEMPLARY CLAIM:        1
NUMBER OF DRAWINGS:     29 Drawing Page(s)
LINE COUNT:             5782
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB      The invention relates to the use of protein design automation (PDA.TM.)
        to generate computationally prescreened secondary libraries of proteins,
        and to methods and compositions utilizing the libraries.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L10  ANSWER 2 OF 3  USPATFULL on STN
ACCESSION NUMBER:       2003:189003  USPATFULL
TITLE:                  Protein modeling tools
INVENTOR(S):            Skolnick, Jeffrey, Creve Corner, MD, UNITED STATES
                        Kolinski, Andrzej, Warsaw, POLAND

                             NUMBER        KIND    DATE
                        ---------------- ------ --------
PATENT INFORMATION:     US 2003130797      A1   20030710            <--
APPLICATION INFO.:      US 2001-982488     A1   20011017  (9)
RELATED APPLN. INFO.:   Division of Ser. No. US 2000-493022, filed on 27 Jan
                        2000, PENDING
```

	NUMBER	DATE	
PRIORITY INFORMATION:	US 1999-117570P	19990127 (60)	<--
	US 1999-118844P	19990205 (60)	<--

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: GREGORY P. EINHORN, Fish & Richardson P.C., Suite 500, 4350 La Jolla Village Drive, San Diego, CA, 92122
NUMBER OF CLAIMS: 13
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 21 Drawing Page(s)
LINE COUNT: 4029

AB The invention provides a new, efficient method for the assembly of protein tertiary structure from known, loosely encoded secondary structure constraints and sparse information about exact side chain contacts. The method is based on a new method for the reduced modeling of protein structure and dynamics, where the protein is described by representing side chain centers of mass rather than alpha-carbons. The model has implicit, built-in multi-body correlations that simulate short- and long-range packing preferences, hydrogen bonding cooperativity, and a mean force potential describing hydrophobic interactions. Due to the simplicity of the protein representation and definition of the model force field, the Monte Carlo algorithm is at least an order of magnitude faster than previously published Monte Carlo algorithms for three-dimensional structure assembly. In contrast to existing algorithms, the new method requires a smaller number of tertiary constraints for successful fold assembly; on average, one for every seven residues as compared to one for every four residues. The reliability and robustness of the invention make it useful for routine application in model building protocols based on various (and even very sparse) experimentally-derived structural constraints.

L10 ANSWER 3 OF 3 USPATFULL on STN
ACCESSION NUMBER: 2003:78520 USPATFULL
TITLE: Novel proteins with integrin-like activity
INVENTOR(S): Mayo, Stephen, Pasadena, CA, UNITED STATES
Shifman, Julia, Pasadena, CA, UNITED STATES
Shimaoka, Motomu, Brookline, MA, UNITED STATES
Springer, Timothy, Newton, MA, UNITED STATES

	NUMBER	KIND	DATE		
PATENT INFORMATION:	US 2003054440	A1	20030320		<--
	US 6951927	B2	20051004		
APPLICATION INFO.:	US 2001-902481	A1	20010709	(9)	

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2000-216600P	20000707 (60)	<--

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: FLEHR, HOHBACH, TEST, ALBRITTON & HERBERT LLP, Suite 3400, Four Embarcadero Center, San Francisco, CA, 94111
NUMBER OF CLAIMS: 30
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 12 Drawing Page(s)
LINE COUNT: 3976
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel proteins with novel integrin and I domain

activity and nucleic acids encoding these proteins. The invention further relates to the use of the novel proteins in the treatment of integrin related disorders.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d ibib abs ind l2 1-1

L2 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:220217 HCAPLUS
DOCUMENT NUMBER: 142:276463
TITLE: Calculating a potential of mean force (PMF) score of a **protein-ligand** complex including a repulsion-term module, and potential drug discovery applications
INVENTOR(S): **Purvis, George D.**
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 9 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005055165	A1	20050310	US 2003-655870	20030905
PRIORITY APPLN. INFO.:			US 2003-655870	20030905

AB To identify a ligand that may have greater binding affinity to a protein associated with the illness, potential mean force (PMF) scores of multiple **protein-ligand** complexes that each include the protein and one of multiple ligands may be calculated and compared with each other. A PMF score of a **protein-ligand** complex may indicate the binding affinity between the protein and ligand. A ligand in a **protein-ligand** complex that has a lower (more neg.) PMF score may be a better candidate for a drug that may be used to treat the illness than a ligand in a **protein-ligand** complex that has a higher PMF score. A system for calculating a PMF score of a **protein-ligand** complex includes a repulsion-term module that accesses parameters usable to calculate a repulsion term usable to calculate a PMF of a **protein-ligand** atom pair in the **protein-ligand** complex. The parameters correspond to an atom-pair type of the **protein-ligand** atom pair. The repulsion-term module uses the accessed parameters to calculate the repulsion term usable to calculate the PMF of the **protein-ligand** atom pair. The repulsion-term module communicates the calculated repulsion term for calcn. of the PMF score of the **protein-ligand** complex.

IC ICM G01N033-48
ICS G01N033-50; G01N031-00
INCL 702019000
CC 9-16 (Biochemical Methods)
Section cross-reference(s): 1, 6
ST **protein ligand** mean force potential repulsion term drug discovery
IT Computer application
Computer program
Drug discovery
Interatomic potential
Molecular association
Molecular mechanics
Molecular modeling
Pair potential
Potential energy
Repulsive potential

(calculating potential of mean force (PMF) score of **protein-ligand** complex including repulsion-term module, and potential drug discovery applications)

IT Ligands
Proteins
RL: PRP (Properties)
(complexes; calculating potential of mean force (PMF) score of **protein-ligand** complex including repulsion-term module, and potential drug discovery applications)

IT Algorithm
(genetic; calculating potential of mean force (PMF) score of **protein-ligand** complex including repulsion-term module, and potential drug discovery applications)

IT Databases
(protein data bank; calculating potential of mean force (PMF) score of **protein-ligand** complex including repulsion-term module, and potential drug discovery applications)